

# Quantum walk, entanglement and thermodynamic laws

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## Abstract

We consider an special dynamics of a quantum walk (QW) on a line. Initially, the walker localized at the origin of the line with arbitrary chirality, evolves to an asymptotic stationary state. In this stationary state a measurement is performed and the state resulting from this measurement is used to start a second QW evolution to achieve a second asymptotic stationary state. In previous works, we developed the thermodynamics associated with the entanglement between the coin and position degrees of freedom in the QW. Here we study the application of the first and second laws of thermodynamics to the process between the two stationary states mentioned above. We show that: i) the entropy change has upper and lower bounds that are obtained analytically as a function of the initial conditions. ii) the energy change is associated to a heat-transfer process.

*Key words:* Quantum thermodynamic; Quantum walk

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## 1 Introduction

Quantum walks (QWs) constitute the quantum analogue of classical random walks [1] and also the quantum version of cellular automata [2]. They have been intensively investigated, especially in connection with quantum information science [3,4,5,6,7,8,9]. As in the classical case, QWs have been proposed as elements to design quantum algorithms [10,11,12,13] and more recently it has been shown that they can be used as a universal model for quantum computation [14,15].

We have been investigating [16,17,18] the asymptotic behavior of the QW on a line, focusing on the probability distribution of chirality independently of position. We showed that this distribution has a stationary long-time limit that

depends on the initial conditions and that it is possible to define a thermodynamic equilibrium between the degrees of freedom of position and chirality [19,20,21,22]. For this equilibrium state we have introduced a temperature concept for an unitary closed system.

On the other hand, the fundamental lower bound of the thermodynamic energy cost of information processing has been a topic of active research [23,24]. On average, the minimum amount of work required to erase 1 bit of information from a memory is  $\kappa T \ln 2$  [25]. In the last decades developments in nano-science have enabled the direct measurement of such minuscule amounts of work for small non-equilibrium thermodynamic systems [26]. At the same time recent advances in technology have opened the possibility of building useful quantum computing devices [27]. Therefore, it seems essential to identify bounds on the thermodynamic energy cost of information processing [28] for these new quantum devices.

In the present paper we study the relationship between the QW thermodynamics and information processing. In particular, we show that it is possible to apply the thermodynamic laws to the QW dynamics after a measurement process. We obtain the upper and lower bound for the asymptotic change of the entanglement entropy. Our result may be thought as complementary to the results presented in Refs. [23,24] where the information content and thermodynamic variables are treated on an equal footing.

The paper is organized as follows. In the next section the usual QW on a line is presented, in the third section the system dynamics with measurement is developed, in the fourth section the entropy change between the asymptotic stationary states is studied, in the fifth section the laws of thermodynamics are applied to the same process. Finally, in the last section we draw some conclusions.

## 2 QW on a line

The composite Hilbert space of the QW is the tensor product  $\mathcal{H}_T \otimes \mathcal{H}_\pm$  where  $\mathcal{H}_T$  is the Hilbert space associated to the motion on a line and  $\mathcal{H}_\pm$  is the chirality (or coin) Hilbert space. In this composite space the walker moves, at discrete time steps  $t \in \mathbb{N}$ , along a one-dimensional lattice of sites  $k \in \mathbb{Z}$ . The direction of motion depends on the chirality states, either right or left. The wave vector can be expressed as the spinor

$$|\Psi(t)\rangle = \sum_{k=-\infty}^{\infty} \begin{pmatrix} a_k(t) \\ b_k(t) \end{pmatrix} |k\rangle, \quad (1)$$

where the upper (lower) component is associated to the left (right) chirality. The QW is ruled by a unitary map whose standard form is [29,30,31,32]

$$\begin{aligned} a_k(t+1) &= a_{k+1}(t) \cos \theta + b_{k+1}(t) \sin \theta, \\ b_k(t+1) &= a_{k-1}(t) \sin \theta - b_{k-1}(t) \cos \theta, \end{aligned} \quad (2)$$

where  $\theta \in [0, \pi/2]$  is a parameter defining the bias of the coin toss. Here we take  $\theta = \frac{\pi}{4}$  for an unbiased or Hadamard coin. The probability of finding the walker at  $(k, t)$  is

$$P(k, t) = |a_k(t)|^2 + |b_k(t)|^2. \quad (3)$$

The global left and right chirality probabilities are defined as

$$\begin{aligned} P_L(t) &\equiv \sum_{k=-\infty}^{\infty} |a_k(t)|^2, \\ P_R(t) &\equiv \sum_{k=-\infty}^{\infty} |b_k(t)|^2, \end{aligned} \quad (4)$$

with  $P_R(t) + P_L(t) = 1$  and the interference term is defined as

$$Q(t) \equiv \sum_{k=-\infty}^{\infty} a_k(t) b_k^*(t). \quad (5)$$

In the generic case  $Q(t)$  together with  $P_L(t)$  and  $P_R(t)$  are time depend functions that have long-time limiting values [16] which are determined both by the initial conditions and by the map in Eq.(2). The relation between the initial condition and the asymptotic distributions has also been recently explored in Ref.[33]. Let us call the mentioned limits as

$$\begin{aligned} \Pi_L &\equiv \lim_{t \rightarrow \infty} P_L(t), \\ \Pi_R &\equiv \lim_{t \rightarrow \infty} P_R(t), \\ Q_0 &\equiv \lim_{t \rightarrow \infty} Q(t) = \mu + i\nu, \end{aligned} \quad (6)$$

where  $\mu$  and  $\nu$  are respectively the real and imaginary part of  $Q_0$ . The following relations are verified [16] between  $\Pi_L$ ,  $\Pi_R$  and  $Q_0$

$$\begin{aligned} \Pi_L &\equiv \frac{1}{2} + \mu, \\ \Pi_R &\equiv \frac{1}{2} - \mu. \end{aligned} \quad (7)$$

It is important to emphasize that the asymptotic behavior in Eq.(6) is determined by the interference term  $Q_0$  that only depends on the initial conditions.

The initial condition the walker localized at the origin with arbitrary chirality will play a central roll in our analytic treatment. Then

$$|\Psi_1(0)\rangle = \begin{pmatrix} \cos(\gamma/2) \\ \exp i\varphi \sin(\gamma/2) \end{pmatrix} |0\rangle, \quad (8)$$

where  $\gamma \in [0, \pi]$  and  $\varphi \in [0, 2\pi]$  define a point on the unit Bloch sphere. We obtain [16]

$$Q_0 = \frac{1}{2} \left(1 - \frac{1}{\sqrt{2}}\right) \left[ \cos \gamma + \sin \gamma (\cos \varphi + i\sqrt{2} \sin \varphi) \right], \quad (9)$$

and also  $\Pi_L$  and  $\Pi_R$  using Eq.(7).

### 3 Dynamical evolution and measurement

#### 3.1 First step

We consider first the QW evolution starting from the initial condition given by Eq.(8) and determine the asymptotic density matrix. The quantum density matrix is defined as

$$\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|, \quad (10)$$

substituting Eq.(1) into Eq.(10) we have

$$\rho(t) = \sum_{k,k'} \begin{pmatrix} a_k(t)a_{k'}^*(t) & a_k(t)b_{k'}^*(t) \\ a_k^*(t)b_{k'}(t) & b_k(t)b_{k'}^*(t) \end{pmatrix} |k\rangle\langle k'|, \quad (11)$$

where  $a_k(t)$  and  $b_k(t)$  depend also on the initial conditions  $\gamma$  and  $\varphi$ .

Note that when  $t \rightarrow \infty$  the limits of  $a_k(t)$  and  $b_k(t)$  are not defined because, in general, they have an oscillatory asymptotic behavior [4]; however the limits given by Eq.(6) are always well defined. In the following we call  $\mathbf{a}_k$  and  $\mathbf{b}_k$  to the values of  $a_k(t)$  and  $b_k(t)$  respectively, evaluated at times large enough so that the asymptotic limit, Eq.(6), is essentially attained.

Let us define the asymptotic reduced density matrix as  $\rho_{1c} = \lim \text{tr}(\rho) =$

$\lim \sum_l \langle l | \rho | l \rangle$  for  $t \rightarrow \infty$ . This matrix takes the following shape

$$\rho_{1c} = \begin{pmatrix} \Pi_L & Q_0 \\ Q_0^* & \Pi_R \end{pmatrix}. \quad (12)$$

### 3.2 Second step

When the asymptotic density matrix is attained a measurement of position and chirality is performed. Then the wave function collapses into one element of the set of eigenvectors of the measurement operator  $\{|k\rangle|\pm\rangle\}$ , where

$$\begin{aligned} |+\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \\ |-\rangle &= \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \end{aligned} \quad (13)$$

After the measurement, the density matrix has the form

$$\rho_1 = \sum_{k=-\infty}^{\infty} |\mathbf{a}_k|^2 |k+\rangle \langle k+| + \sum_{k=-\infty}^{\infty} |\mathbf{b}_k|^2 |k-\rangle \langle k-|, \quad (14)$$

where  $|k\pm\rangle = |k\rangle|\pm\rangle$ . Eq.(14) can be written in matrix form as

$$\rho_1 \equiv \sum_k \begin{pmatrix} |\mathbf{a}_k|^2 & 0 \\ 0 & |\mathbf{b}_k|^2 \end{pmatrix} |k\rangle \langle k|. \quad (15)$$

Equation (14) sets a new initial condition and we will study the asymptotic evolution of the new density matrix. Essentially we must study the evolution of the densities  $|k\pm\rangle \langle k\pm|$ . We know, from the QW dynamics, that if the initial condition is given by Eq.(8) then the density matrix is given by Eq.(11). We can use these equations as a recipe to obtain the unknown evolutions, that is, when we choose a particular initial condition given by  $|k\pm\rangle$  we have

$$\begin{aligned} U(t)|k\pm\rangle \langle k\pm| U^\dagger(t) = \\ \sum_{n,n'} \begin{pmatrix} a_{n\pm}(t,k) a_{n'\pm}^*(t,k) & a_{n\pm}(t,k) b_{n'\pm}^*(t,k) \\ a_{n^*\pm}(t,k) b_{n'\pm}(t,k) & b_{n\pm}(t,k) b_{n'\pm}^*(t,k) \end{pmatrix} |n\rangle \langle n'|, \end{aligned} \quad (16)$$

where  $U(t)$  is the QW evolution operator and  $a_{n\pm}(t,k)$  and  $b_{n\pm}(t,k)$  verify the map Eq.(2), that is  $a_{n\pm}(t,k)$  and  $b_{n\pm}(t,k)$  are equivalent to some functions  $a_n(t)$  and  $b_n(t)$ . The expressions  $a_{n\pm}(t,k)$  and  $b_{n\pm}(t,k)$  show explicitly their

dependence both on the chirality,  $\{|+\rangle, |-\rangle\}$ , as with,  $k$ , the walker's initial position on a line. Therefore, the new quantum density matrix is

$$\begin{aligned}\rho(t) &= U(t)\rho_1 U^\dagger(t) \\ &= \sum_{n,n'} \begin{pmatrix} A_{11}(n, n') & A_{12}(n, n') \\ A_{21}(n, n') & A_{22}(n, n') \end{pmatrix} |n\rangle \langle n'|, \end{aligned} \quad (17)$$

where

$$\begin{aligned}A_{11}(n, n') &= \sum_k \left[ |\mathbf{a}_k|^2 a_{n+}(t, k) a_{n'+}^*(t, k) \right. \\ &\quad \left. + |\mathbf{b}_k|^2 a_{n-}(t, k) a_{n'-}^*(t, k) \right], \end{aligned} \quad (18)$$

$$\begin{aligned}A_{22}(n, n') &= \sum_k \left[ |\mathbf{a}_k|^2 b_{n+}(t, k) b_{n'+}^*(t, k) \right. \\ &\quad \left. + |\mathbf{b}_k|^2 b_{n-}(t, k) b_{n'-}^*(t, k) \right], \end{aligned} \quad (19)$$

$$\begin{aligned}A_{12}(n, n') &= \sum_k \left[ |\mathbf{a}_k|^2 a_{n+}(t, k) b_{n'+}^*(t, k) \right. \\ &\quad \left. + |\mathbf{b}_k|^2 a_{n-}(t, k) b_{n'-}^*(t, k) \right], \end{aligned} \quad (20)$$

$$A_{21}(n, n') = A_{12}^*(n, n'). \quad (21)$$

We again point out that the probability density has an asymptotic limit for long times. We now call the values of  $a_{n\pm}(t, k)$  and  $b_{n\pm}(t, k)$  evaluated at such times  $\mathbf{a}_{n\pm}(k)$  and  $\mathbf{b}_{n\pm}(k)$  respectively. We want to calculate in this limit the reduced density matrix, namely  $\rho_{2c} = \lim \text{tr}(\rho) = \lim \sum_l \langle l | \rho | l \rangle$ ,  $t \rightarrow \infty$ . Using the density matrix given by Eq.(17), we have

$$\begin{aligned}\rho_{2c} &= \lim_{t \rightarrow \infty} \sum_{l=-\infty}^{\infty} \begin{pmatrix} A_{11}(l, l) & A_{12}(l, l) \\ A_{12}^*(l, l) & A_{22}(l, l) \end{pmatrix}, \end{aligned} \quad (22)$$

where

$$\begin{aligned}\lim_{t \rightarrow \infty} \sum_{l=-\infty}^{\infty} A_{11}(l, l) &= \sum_k |\mathbf{a}_k|^2 \sum_l |\mathbf{a}_{l+}(k)|^2 \\ &\quad + \sum_k |\mathbf{b}_k|^2 \sum_l |\mathbf{a}_{l-}(k)|^2, \end{aligned} \quad (23)$$

$$\begin{aligned}
\lim_{t \rightarrow \infty} \sum_{l=-\infty}^{\infty} A_{12}(l, l) &= \sum_k |\mathbf{a}_k|^2 \sum_l \mathbf{a}_{l+}(k) \mathbf{b}_{l+}^*(k) \\
&+ \sum_k |\mathbf{b}_k|^2 \sum_l \mathbf{a}_{l-}(k) \mathbf{b}_{l-}^*(k),
\end{aligned} \tag{24}$$

$$\begin{aligned}
\lim_{t \rightarrow \infty} \sum_{l=-\infty}^{\infty} A_{22}(l, l) &= \sum_k |\mathbf{a}_k|^2 \sum_l |\mathbf{b}_{l+}(k)|^2 \\
&+ \sum_k |\mathbf{b}_k|^2 \sum_l |\mathbf{b}_{l-}(k)|^2.
\end{aligned} \tag{25}$$

According to Eqs.(4), (5) and (6), we define

$$\Pi_{L\pm} \equiv \sum_l |\mathbf{a}_{l\pm}(k)|^2, \tag{26}$$

$$\Pi_{R\pm} \equiv \sum_l |\mathbf{b}_{l\pm}(k)|^2, \tag{27}$$

$$Q_{0\pm} \equiv \sum_l \mathbf{a}_{l\pm}(k) \mathbf{b}_{l\pm}^*(k). \tag{28}$$

To obtain the explicit shape of  $\Pi_{L\pm}$ ,  $\Pi_{R\pm}$  and  $Q_{0\pm}$ , we can use again Eqs.(7, 9) where the initial condition is, the walker localized at the position  $k$  with chirality  $|\pm\rangle$  respectively, *i.e.*

$$|\Psi_{2\pm}(0)\rangle = |\pm\rangle|k\rangle. \tag{29}$$

Note that the principal difference between Eq.(8) and Eq.(29) is in the walker's initial position, that is, in Eq.(29)  $k$  is arbitrary and in Eq.(8)  $k = 0$ . However, even with this difference, Eq.(5) continues to be valid for the calculation of  $Q_{0\pm}$  because the original map, Eq.(2), is invariant under translations and therefore this magnitude is independent of  $k$ . For the same reason Eqs.(26) and (27) are independent of  $k$ , and then Eq. (22) reduces to

$$\rho_{2c} = \Pi_L \rho_L + \Pi_R \rho_R, \tag{30}$$

where

$$\rho_L = \begin{pmatrix} \Pi_{L+} & Q_{0+} \\ Q_{0+}^* & \Pi_{R+} \end{pmatrix}, \tag{31}$$

$$\rho_R = \begin{pmatrix} \Pi_{L-} & Q_{0-} \\ Q_{0-}^* & \Pi_{R-} \end{pmatrix}, \tag{32}$$

and  $\Pi_L$  and  $\Pi_R$  are given by Eqs.(7, 9). Moreover, using the initial condition of Eq.(29) in Eq.(9) and Eq.(7) it is straightforward to obtain

$$\begin{aligned} Q_{0+} &= -Q_{0-} = \frac{1}{2} - \frac{1}{2\sqrt{2}}, \\ \Pi_{L+} &= \Pi_{R-} = 1 - \frac{1}{2\sqrt{2}}, \\ \Pi_{R+} &= \Pi_{L-} = \frac{1}{2\sqrt{2}}. \end{aligned} \quad (33)$$

Note that  $\rho_L$  and  $\rho_R$ , Eqs.(31, 32), are the asymptotic densities that correspond to initial conditions associated with the eigenvalues  $|+\rangle$  and  $|-\rangle$  respectively. Therefore, Eq.(30) has a natural interpretation, after the measurement the asymptotic reduced density matrix is the weighted average of the two densities associated with the two possible values of the chirality.

## 4 Entropy change

The unitary evolution of the QW generates entanglement between the coin and position degrees of freedom which can be quantified through the associated von Neumann entropy. This entropy of entanglement is defined by the reduced density operator

$$S(\rho_c) = -\kappa \operatorname{tr}(\rho_c \log \rho_c), \quad (34)$$

where  $\kappa$  denotes a proportionality constant, the Boltzmann constant.

For a pure state the minimum entropy  $S(\rho_c) = 0$  is attained. The maximum entropy (or minimum purity) is to be found for the broadest possible probability distribution, the equipartition over all pure states.

Equation (34) can be expressed as a function of the eigenvalues of  $\rho_c$ ,  $\Lambda_+$  and  $\Lambda_-$

$$\frac{S(\rho_c)}{\kappa} = -\Lambda_+ \log \Lambda_+ - \Lambda_- \log \Lambda_-. \quad (35)$$

Using Eqs.(12), (30), (31) and (32) we can calculate the entanglement entropies for the four stationary densities introduced in the previous section. The eigenvalues of the density operator  $\rho_{1c}$  are

$$\Lambda_{1\pm} = \frac{1}{2} \pm \sqrt{2\mu^2 + \nu^2}, \quad (36)$$

and those of  $\rho_{2c}$  are

$$\Lambda_{2\pm} = \frac{1}{2} \pm |\mu|(\sqrt{2} - 1). \quad (37)$$



The operators  $\rho_L$  and  $\rho_R$  have the same eigenvalues and they are

$$\Lambda_{LR\pm} = \frac{1}{2} \mp \frac{1}{2} \sqrt{3 - \frac{3}{\sqrt{2}}}. \quad (38)$$

Therefore, the four entanglement entropies are expressed as

$$\frac{S(\rho_{1c})}{\kappa} = -\Lambda_{1+} \log \Lambda_{1+} - \Lambda_{1-} \log \Lambda_{1-}, \quad (39)$$

$$\frac{S(\rho_{2c})}{\kappa} = -\Lambda_{2+} \log \Lambda_{2+} - \Lambda_{2-} \log \Lambda_{2-}, \quad (40)$$

$$\frac{S(\rho_L)}{\kappa} = -\Lambda_{LR+} \log \Lambda_{LR+} - \Lambda_{LR-} \log \Lambda_{LR-}, \quad (41)$$

$$\frac{S(\rho_R)}{\kappa} = \frac{S(\rho_L)}{\kappa} \approx 0.139. \quad (42)$$

We now show that  $S(\rho_{2c})$  has a non obvious upper bound, using a known theorem that plays an important role in many applications of quantum information theory [34]. Applying the mentioned theorem to the entropy of the mixture of quantum states given by Eq. (30), the following upper bound is obtained

$$S_2 \equiv S(\rho_L) - \kappa (\Pi_L \log \Pi_L + \Pi_R \log \Pi_R) \geq S(\rho_{2c}). \quad (43)$$

The entropies  $S(\rho_{1c})$ ,  $S(\rho_{2c})$  and the expression  $S_2$  only depend on the interference term  $Q_0$ .

Note that from Eq.(9) we have  $|Q_0| \leq \frac{1}{2}(1 - \frac{1}{\sqrt{2}}) < 1$ , then we approximate the log functions in Eqs. (39), (40) and (43), using the first few terms of their Taylor series to calculate the entropy change between the two asymptotic stationary states,

$$\frac{S(\rho_{2c}) - S(\rho_{1c})}{\kappa} \approx 2\nu^2 + 2(2\sqrt{2} - 1)\mu^2. \quad (44)$$

The distance between  $S(\rho_{2c})$  and its upper bound can be approximated by

$$\frac{S_2 - S(\rho_{2c})}{\kappa} \approx \frac{S(\rho_L)}{\kappa} - 4(\sqrt{2} - 1)\mu^2. \quad (45)$$

Combining Eqs.(43), (44) and (45), it is easy to obtain the following upper bound for  $S(\rho_{2c}) - S(\rho_{1c})$

$$J_1 \equiv S(\rho_L) + 2\kappa(\mu^2 + \nu^2) \geq S(\rho_{2c}) - S(\rho_{1c}). \quad (46)$$

When  $Q_0$  vanishes, Eq.(44) shows that  $S(\rho_{1c}) = S(\rho_{2c})$  and these entropies take their maximum value. Moreover in this case ( $Q_0 = 0$ ) the QW dynamics can be described as a classical Markovian process [30]; it has a Markovian

behavior both before and after the measurement. The initial conditions for this behavior are  $\gamma = -\pi/4, \pi/4$  and  $\varphi = 0, \pi$  respectively. When  $Q_0 \neq 0$ , the measurement process essentially determines an entropy increase for the system,  $S(\rho_{2c}) - S(\rho_{1c}) > 0$ .

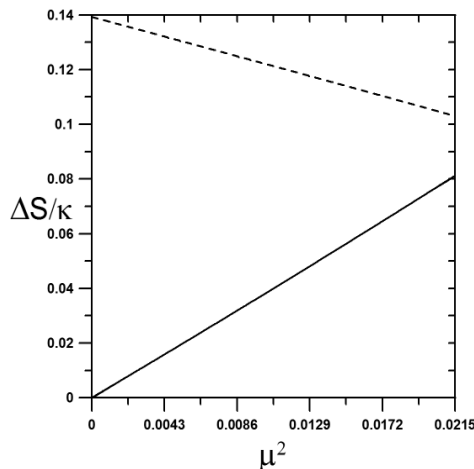


Fig. 1. Dimensionless entropy change as a function of  $|Q_0|^2 = \mu^2$  for the case  $\varphi = 0$ . In thick line the entropy change given by Eq.(44). In dashed line the entropy change given by Eq.(45).

The entropy change for a real  $Q_0$  is depicted in Fig. 1. The calculation was made using the entropy definition Eqs. (39, 40, 41, 42), therefore the curves show that the lineal approximation proposed in Eqs. (44, 45) is excellent.

## 5 Thermodynamic laws.

In previous works [19,20,21,22], we studied the behavior of the chirality distribution and we introduced the temperature concept for an unitary closed system. In this theory one considers the system associated with the chirality degrees of freedom and described by  $\rho_c$ , interacting through its entanglement with the position degrees of freedom, the lattice, as equivalent to the thermal contact with a bath. Therefore, in equilibrium

$$[H_c, \rho_c] = 0, \quad (47)$$

should be satisfied, where  $H_c$  is the interaction Hamiltonian between the chirality and the lattice. In the QW case, the explicit shape of  $H_c$  is unknown for us, however we know that the eigenvalues of  $H_c$  are independent of the initial condition of the wave function, they only depend on the unitary evolution. In contrast, the eigenvalues  $\Lambda_{\pm}$  depend on the initial conditions and the corresponding eigenvalues of  $H_c$ . We call  $\{|\Phi_{\pm}\rangle\}$  the set of eigenfunctions common to the density matrix and the Hamiltonian, then in this basis the operators  $\rho_c$

and  $H_c$  are both diagonal. Moreover, since only the relative difference between energy eigenvalues has physical significance, we denote this set of eigenvalues by  $\pm\epsilon$ ; they may be interpreted as the possible values of the entanglement energy. This interpretation agrees with the fact that  $\Lambda_{\pm}$  is the probability that the system is in the eigenstate  $|\Phi_{\pm}\rangle$ .

The precise dependence between  $\Lambda_{\pm}$  and  $\pm\epsilon$  is determined by the type of ensemble we construct. We propose that our equilibrium state corresponds to a quantum canonical ensemble. To this end we set

$$\Lambda_{\pm} \equiv \frac{e^{\mp\beta\epsilon}}{\mathcal{Z}}, \quad (48)$$

where  $\mathcal{Z}$  is the partition function of the system, that is

$$\mathcal{Z} \equiv e^{-\beta\epsilon} + e^{\beta\epsilon}, \quad (49)$$

and the parameter  $\beta$  can be put into correspondence with an entanglement temperature

$$T \equiv \frac{1}{\kappa\beta} = \frac{-2\epsilon}{\kappa \log(\Lambda_+/\Lambda_-)}. \quad (50)$$

The entanglement temperature, Eq.(50), can take any finite, infinite, positive or negative value. Note that when the energy of a system is bounded from above there is no compelling reason to exclude the possibility of negative temperatures.

In this statistical mechanics frame it is possible to define the internal energy of entanglement between the coin and position degrees of freedom

$$U(\rho) = \epsilon\Lambda_+ - \epsilon\Lambda_-. \quad (51)$$

The variations of temperature,  $\Delta T$  and internal energy,  $\Delta U$  between the two asymptotic states can be calculated as functions of the interference term  $Q_0$ . Using Eqs.(36) and (37) together with Eqs.(50) and (51) we have

$$\begin{aligned} \frac{2\kappa\Delta T}{\epsilon} &= \frac{4}{\log(\Lambda_{1+}/\Lambda_{1-})} - \frac{4}{\log(\Lambda_{2+}/\Lambda_{2-})} \\ &\simeq \frac{1}{\sqrt{2\mu^2 + \nu^2}} - \frac{1}{(\sqrt{2} - 1)|\mu|}, \end{aligned} \quad (52)$$

$$\frac{\Delta U}{2\epsilon} = (\sqrt{2} - 1)|\mu| - \sqrt{2\mu^2 + \nu^2}. \quad (53)$$

Equation (52) shows that  $\Delta T = 0$  is only possible if  $\Lambda_{1+}\Lambda_{2-} = \Lambda_{1-}\Lambda_{2+}$ , and this implies that  $Q_0 = 0$ , then the two asymptotic states have the same temperature and in this sense we can think of an “isothermal process”. As the temperature concept makes sense only in an equilibrium state it is clear

that between these two asymptotic states the temperature is not defined. Additionally Eq.(53) implies that  $\Delta U \leq 0$  and vanishes when  $Q_0 = 0$ .

The first law of thermodynamics is now applied to the evolution between the two asymptotic stationary states expressed as

$$\Delta U = \mathcal{Q} + \mathcal{W}, \quad (54)$$

where  $\mathcal{Q}$  is the QW heat absorbed during the measurement process and  $\mathcal{W}$  is the work made over the QW. Thermodynamic work is defined to be measurable solely from the knowledge of external constraint variables. In this system the only parametric dependence of the thermodynamical functions is with the temperature, because the energy levels  $\{-\epsilon, \epsilon\}$  are maintained constant, then  $\mathcal{W} = 0$ . Therefore the first law is reduced to

$$\Delta U = \mathcal{Q}. \quad (55)$$

From Eq.(55) we conclude that: i) The change of internal energy is due to the heat delivered during the measurement process. ii) The heat behaves as a state function, then the real process can be substituted by a quasi-static process between the two asymptotic stationary states (characterized by their temperatures), where it is possible to defined the infinitesimal  $d\mathcal{Q}$ .

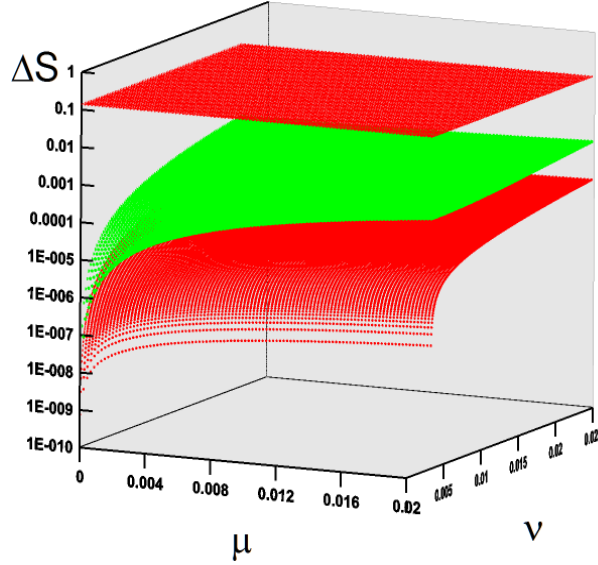


Fig. 2. (Color on line) The dimensionless entropy change (in log scale) as a function of the dimensionless interference term  $Q_0 = \mu + i\nu$ . The medium (green) surface is the change of entropy given by Eq.(44). The upper and lower (red) surfaces are the upper and lower bounds  $J_1$  and  $J_2$  given by Eq.(46) and Eq.(59) respectively.

In general, for an irreversible process, the second law of thermodynamics is expressed as

$$\Delta S > \int \frac{d\mathcal{Q}}{T}. \quad (56)$$

The question may be posed if this law is satisfied for the entropy, temperature and heat that were defined in our system. The answer to this question must be positive because the starting point of our theory has been to postulate the canonical distribution for the reduced density matrix therefore the thermodynamic laws are obeyed. We do not know the temperature dependence with the absorbed heat in order to compute the integral in Eq.(56). However we can obtain a bound for this integral in order to verify the second law for the entanglement between the coin and position degrees of freedom. We have  $|T_1| < |T_2|$ , where  $T_1$  and  $T_2$  are the temperatures of the stationary states before and after the measurement. Then

$$J_2 \equiv \frac{Q}{T_2} \leq \int \frac{dQ}{T} < S(\rho_{2c}) - S(\rho_{1c}). \quad (57)$$

Therefore, using Eq.(55) we can propose the second law for the entanglement entropy

$$S(\rho_{2c}) - S(\rho_{1c}) > J_2 = \frac{\Delta U}{T_2} \geq 0. \quad (58)$$

The lower bound  $J_2$  can be expressed as a function of the interference term  $Q_0$ , Eqs.(36, 37, 50, 53, 55, 58)

$$\frac{J_2}{\kappa} \simeq (\sqrt{2} - 1) |\mu| \left[ \sqrt{2\mu^2 + \nu^2} - (\sqrt{2} - 1) |\mu| \right]. \quad (59)$$

In Fig. 2 we show the entropy change together with its bounds. The entropy calculations were made using the definitions Eqs. (39, 40). We conclude that the second law of thermodynamic in the form of Eq.(58) is satisfied by the theory developed in the present paper and additionally we show the correctness of the upper bound given by equation Eq.(46).

## 6 Conclusion

In previous works we developed the thermodynamics associated with the entanglement between the coin and position degrees of freedom. Here we consider a special dynamics of a QW on a line. Initially, the walker localized at the origin with arbitrary chirality, evolves to an asymptotic stationary state, then a measurement is performed and the state resulting from this measurement is the initial condition for a second QW dynamics to achieve a second asymptotic stationary state.

We have studied the first and second laws of thermodynamics in the process between the two stationary states mentioned before. These asymptotic stationary states only depends on the initial conditions through the interference

term of the initial wave function. We show that the change of entropy has upper and lower bounds and they are obtained analytically as a function of the initial conditions. We have also shown that the measurement process changes the energy and this change is associated to a heat transference process.

Moreover, we prove that, if the interference term vanishes the thermodynamics functions of the asymptotic stationary states do not change.

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- [34] see Ref. [28] p. 518: “Suppose  $\rho = \sum_i p_i \rho_i$ , where  $p_i$  are some set of probabilities, and the  $\rho_i$  are density operators. Then

$$S(\rho) \leq -\kappa \sum_i p_i \log p_i + \sum_i p_i S(\rho_i), \quad (60)$$

with equality if and only if the states  $\rho_i$  have support on orthogonal subspaces”.